REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY) 16-08-2018	2. REPORT TYPE Final Report	3. DATES COVERED (From - To) 28-May-2015 - 27-Jul-2018

4. TITLE AND SUBTITLE Final Report: 3.4 Development and Application of High Order Accurate Algorithms	5a. CONTRACT NUMBER W911NF-15-1-0226
	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER 611102

6. AUTHORS	5d. PROJECT NUMBER
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES Brown University Office of Sponsored Projects Box 1929 Providence, RI 02912 -9093	8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES) U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211	10. SPONSOR/MONITOR'S ACRONYM(S) ARO
	11. SPONSOR/MONITOR'S REPORT NUMBER(S) 66192-MA.24

12. DISTRIBUTION AVAILILITY STATEMENT

Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON Chi-Wang Shu
a. REPORT UU	b. ABSTRACT UU	c. THIS PAGE UU	UU		19b. TELEPHONE NUMBER 401-863-2549

Agency Code:

Proposal Number: 66192MA **Agreement Number: W911NF-15-1-0226**

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Country: USA
DUNS Number: 001785542 EIN: 050258809
Report Date: 27-Oct-2018 Date Received: 16-Aug-2018
Final Report for Period Beginning 28-May-2015 and Ending 27-Jul-2018
Title: 3.4 Development and Application of High Order Accurate Algorithms
Begin Performance Period: 28-May-2015 **End Performance Period:** 27-Jul-2018
Report Term: 0-Other
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Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: 1 **STEM Participants:** 2

Major Goals: The goal of this project is to help obtaining more robust, cost effective, and reliable numerical tools for solving problems in physical applications, such as computational fluid dynamics, traffic and pedestrian flow models, cosmological turbulent flows, and optimal control. An emphasis during the proposed work period is on a study of new computational methodologies, to improve the range of applicability, efficiency, and robustness of the proposed methods for various physical problems. Attention is paid to army related applications.

Accomplishments: Research has been performed and results obtained in the following directions in order to reach the major goals:

Based on the recently developed fifth order WENO schemes which improve the convergence of the classical WENO schemes by removing slight post-shock oscillations, we have designed fifth order fixed-point sweeping WENO methods for efficient computation of steady state solution of hyperbolic conservation laws.

A local Riemann solver for strongly nonlinear equations of state (EOS) is presented, which has suppressed successfully numerical oscillation caused by high-density ratio and high-pressure ratio across the interface between explosion products and air. A fifth order finite difference weighted essentially non-oscillatory (WENO) scheme has been developed to realize the parallel simulation of three-dimensional (3D) air explosion. The overall process of 3D air explosion of both TNT and aluminized explosives has been successfully simulated.

A maximum-principle-satisfying Space-Time Conservation Element and Solution Element (CE/SE) scheme is constructed, focusing on its application to a reduced five-equation model coupled with the stiffened equation of state for compressible multifluids. The present scheme can sharply capture shocks and interfaces and strictly confine the volume fraction of each component in its range, and has good conservativeness and can derive pressure-oscillation-free results across the interface separating two fluids with large difference of densities and thermodynamic properties.

We have analyzed the stability of the fourth order Runge-Kutta method for integrating semi-discrete approximations of time-dependent partial differential equations. A counter example is given to show that the classical four-stage fourth order Runge-Kutta method can not preserve the one-step strong stability, but with an energy argument, we show that the strong stability property holds in two steps. Since the classical fourth order Runge-Kutta method is used extensively in applications, the results in this work provide important theoretical guidance about its stability properties.

We have developed a local discontinuous Galerkin (LDG) method to solve 2D Keller-Segel (KS) chemotaxis model, which describes cell movements and flocking phenomena, and give optimal rate of convergence under special finite element spaces before the blow-up occurs.

We have constructed a new type of finite difference Hermite weighted essentially non-oscillatory (HWENO) schemes for solving Hamilton-Jacobi (HJ) equations, which have important applications in computational fluid dynamics and control.   The main advantages of this new scheme include its compactness in the spatial field and its simplicity in the reconstructions.

We have proposed a simple bound-preserving sweeping procedure for conservative numerical approximations, which has a very general framework acting as a postprocessing step accommodating many point-based or cell average-based discretizations. The technique is demonstrated to work well with a spectral method, high order finite difference and finite volume methods for scalar conservation laws and incompressible flows.

We have introduced a new troubled-cell indicator for the mdiscontinuous Galerkin (DG) methods for solving hyperbolic conservation laws. This indicator can be defined on unstructured meshes for high order DG methods and depends only on data from the target cell and its immediate neighbors. It is able to identify shocks without PDE sensitive parameters to tune.

We have developed a new class of high order weighted essentially non-oscillatory (WENO) schemes which can remove the usual slight post-shock oscillations and ensure the residue to settle down to machine zero in steady state simulations, for our extensive list of test problems including shocks, contact discontinuities, rarefaction waves or their interactions, and with these complex waves passing through the boundaries of the computational domain. This is a significant advance for steady state computation of high order schemes for shocked flows.

We have designed a high order Lagrangian scheme in cylindrical coordinates, which can maintain both spherical symmetry-preservation and positivity-preservation simultaneously.

We have designed high order positivity-preserving limiter and a simple WENO limiter for a stable, conservative and high order accurate method, based on the discontinuous Galerkin framework, the Voronoi technique and a grouping algorithm, in solving one and two dimensional hyperbolic conservation laws on arbitrarily distributed point clouds. This method has a good potential in applications in which the points of observation and required solution are predetermined and irregular.

We have introduced a definition of the local conservation property for numerical methods solving time dependent conservation laws, which generalizes the classical local conservation definition. Several numerical methods, including continuous Galerkin methods and compact schemes, which do not fit the classical local conservation definition, are given as examples of locally conservative methods under our generalized definition.

We have developed a high-order positivity-preserving DG method with the backward Euler time discretization for conservation laws. Both the analysis and numerical experiments indicate that a lower bound for the CFL number is required to obtain the positivity-preserving property. The proposed scheme not only preserves the positivity of the numerical approximation without compromising the designed high-order accuracy, but also helps accelerate the convergence towards the steady-state solution and add robustness to the nonlinear solver.

We have developed a discontinuous Galerkin (DG) scheme with suitable quadrature rules for ideal compressible magnetohydrodynamic (MHD) equations. The semi-discrete scheme is analyzed to be entropy stable by using the symmetrizable version of the equations as introduced by Godunov. The entropy stability enhances the robustness of the algorithm, as demonstrated by numerical experiments.

We have developed bound-preserving modified exponential Runge-Kutta (RK) discontinuous Galerkin (DG) schemes to solve scalar hyperbolic equations with stiff source terms. Exponential strong stability preserving (SSP) high order time discretizations are constructed and then modified to overcome the stiffness and preserve the bound of the numerical solutions.

We have constructed arbitrarily high order accurate DG schemes which preserve positivity of the radiative intensity in the simulation of both steady and unsteady radiative transfer equations in one- and two-dimensional geometry, by introducing an augmented DG space to ensure positivity of cell averages and then applying the scaling positivity-preserving limiter.

We have developed the discontinuous Galerkin (DG) methods on triangular meshes for solving metamaterial Maxwell's equations. The DG schemes are proved to be stable, energy conserving, and high order accurate. Simulations of wave propagation in Drude metamaterials demonstrate the good performance of the DG methods on triangular meshes.

We have developed a model and an algorithm for simulating the dispersion of vehicle exhaust in a hypothetical city with a single central business district (CBD) in a complete day, deriving an average pollutant concentration in a day, then use the distribution of wind direction in a year, to compute the distribution of average pollutant concentration in the city. This would provide a useful tool for city planning.

We have developed uniformly high-order discontinuous Galerkin (DG) schemes which provably preserve the positivity of density and pressure for multidimensional ideal MHD, using the locally divergence-free DG schemes for the symmetrizable ideal MHD equations.

Training Opportunities: The 7 post-prelim Ph.D. students and 1 postdoc of the PI have benefited from group meetings and discussion sessions, and one Ph.D. student is directly supported by this grant.

Results Dissemination: 23 refereed journal papers (appeared or accepted), and 9 preprints submitted to refereed journals for possible publication, have cited partial support from this grant. The PI and his students / postdoc have attended several international conferences to communicate their results to their scientific colleagues. For example, the PI attended the Oberwolfach Workshop on Recent Developments in the Numerics of Nonlinear Hyperbolic Conservation Laws in Germany in September 2015 to report results related to this project on high order numerical methods.

Published (or accepted) refereed journal papers which have cited partial support from this grant:

[1] L. Wu, Y.-T. Zhang, S. Zhang and C.-W. Shu, High order fixed-point sweeping WENO methods for steady state of hyperbolic conservation laws and its convergence study, Communications in Computational Physics, v20 (2016), pp.835-869.

[2] C.-W. Shu, High order WENO and DG methods for time-dependent convection-dominated PDEs: a brief survey of several recent developments, Journal of Computational Physics, v316 (2016), pp.598-613.

[3] C. Wang, J. Ding, C.-W. Shu and T. Li, Three-dimensional high order large-scale numerical investigation on the air explosion, Computers and Fluids, v137 (2016), pp.70-79.

[4] D.S. Balsara, S. Garain and C.-W. Shu, An efficient class of WENO schemes with adaptive order, Journal of Computational Physics, v326 (2016), pp.780-804.

[5] H. Shen, C.-Y. Wen, M. Parsani and C.-W. Shu, Maximum-principle-satisfying space-time conservation element and solution element scheme applied to compressible multifluids, Journal of Computational Physics, v330 (2017), pp.668-692.

[6] Z. Sun and C.-W. Shu, Stability of the fourth order Runge-Kutta method for time-dependent partial differential equations, Annals of Mathematical Sciences and Applications, v2 (2017), pp.255-284.

[7] X.H. Li, C.-W. Shu and Y. Yang, Local discontinuous Galerkin method for the Keller-Segel chemotaxis model, Journal of Scientific Computing, v73 (2017), pp.943-967.

[8] F. Zheng, C.-W. Shu and J. Qiu, Finite difference Hermite WENO schemes for the Hamilton-Jacobi equations, Journal of Computational Physics, v337 (2017), pp.27-41.

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[10] G. Fu and C.-W. Shu, A new trouble-cell indicator for discontinuous Galerkin methods for hyperbolic conservation laws, Journal of Computational Physics, v347 (2017), pp.305-327.

[11] J. Zhu and C.-W. Shu, Numerical study on the convergence to steady state solutions of a new class of high order WENO schemes, Journal of Computational Physics, v349 (2017), pp.80-96.

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[13] J. Du and C.-W. Shu, Positivity-preserving high-order schemes for conservation laws on arbitrarily distributed point clouds with a simple WENO limiter, International Journal of Numerical Analysis and Modeling, v15 (2018), pp.1-25.

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[15] T. Qin and C.-W. Shu, Implicit positivity-preserving high order discontinuous Galerkin methods for conservation laws, SIAM Journal on Scientific Computing, v40 (2018), pp.A81-A107.

[16] Y. Liu, C.-W. Shu and M. Zhang, Entropy stable high order discontinuous Galerkin methods
for ideal compressible MHD on structured meshes, Journal of Computational Physics, v354 (2018), pp.163-178.

[17] J. Huang and C.-W. Shu, Bound-preserving modified exponential Runge-Kutta discontinuous Galerkin
methods for scalar hyperbolic equations with stiff source terms, Journal of Computational Physics, v361 (2018), pp.
111-135.

[18] D. Ling, J. Cheng and C.-W. Shu, Conservative high order positivity-preserving discontinuous
Galerkin methods for linear hyperbolic and radiative transfer equations, Journal of Scientific Computing, to appear.

[19] H. Wang, Q. Zhang and C.-W. Shu, Third order implicit-explicit Runge-Kutta local discontinuous
Galerkin methods with suitable boundary treatment for convection-diffusion problems with Dirichlet boundary
conditions, Journal of Computational and Applied Mathematics, v342 (2018), pp.164-179.

[20] C. Shi, J. Li and C.-W. Shu, Discontinuous Galerkin methods for Maxwell's equations in Drude metamaterials
on unstructured meshes, Journal of Computational and Applied Mathematics, v342 (2018), pp.147-163.

[21] J. Zhu and C.-W. Shu, Numerical study on the convergence to steady state solutions of a new class of finite
volume WENO schemes: triangular meshes, Shock Waves, to appear.

[22] L. Yang, T. Li, S.C. Wong, C.-W. Shu and M. Zhang, Modeling and simulation of urban air pollution from the
dispersion of vehicle exhaust: a continuum modeling approach, International Journal of Sustainable Transportation,
to appear.

[23] K. Wu and C.-W. Shu, Provably positive discontinuous Galerkin methods for multidimensional ideal
magnetohydrodynamics, SIAM Journal on Scientific Computing, to appear.

Preprints which have cited partial support from this grant:

[1] H. Wang, Q. Zhang, S. Wang and C.-W. Shu, Local discontinuous Galerkin methods with explicit-implicit-null
time discretizations for solving nonlinear diffusion problems, submitted to Science China Mathematics.

[2] L. Zhou, Y. Xia and C.-W. Shu, Stability analysis and error estimates of arbitrary Lagrangian-Eulerian
discontinuous Galerkin method coupled with Runge-Kutta time-marching for linear conservation laws, submitted to
ESAIM: Mathematical Modelling and Numerical Analysis ($M^{2}AN$).

[3] G. Fu and C.-W. Shu, Optimal energy-conserving discontinuous Galerkin methods for linear symmetric
hyperbolic systems, submitted to Journal of Computational Physics.

[4] G. Fu and C.-W. Shu, An energy-conserving ultra-weak discontinuous Galerkin method for
the generalized Korteweg-De Vries equation, submitted to Journal of Computational and Applied Mathematics.

[5] A. Mazaheri, C.-W. Shu and V. Perrier, Bounded and compact weighted essentially nonoscillatory limiters for
discontinuous Galerkin schemes: triangular elements, submitted to Journal of Computational Physics.

[6] J. Huang and C.-W. Shu, Positivity-preserving time discretizations for production-destruction
equations with applications to non-equilibrium flows, submitted to Journal of Scientific Computing.

[7] Y. Liu, Q. Liu, Y. Liu, C.-W. Shu and M. Zhang, Locally divergence-free spectral-DG methods for ideal
magnetohydrodynamic equations on cylindrical coordinates, submitted to Communications in Computational
Physics.

[8] J. Zhu and C.-W. Shu, A new type of multi-resolution WENO schemes with increasingly higher order of
accuracy, submitted to Journal of Computational Physics.

[9] K. Wu and C.-W. Shu, Provably positive high-order schemes for ideal magnetohydrodynamics: analysis on
general meshes, submitted to Mathematical Models and Methods in Applied Sciences.

Honors and Awards: The PI was awarded an Honorary Fellowship by the European Society of Computational Methods in Sciences and Engineering, in Greece, in September 2016.

Protocol Activity Status:

Technology Transfer: The algorithms designed by the PI have been used by DoD scientists including army lab scientists.

PARTICIPANTS:

Participant Type: PD/PI
Participant: Chi-Wang Shu
Person Months Worked: 5.00   **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Nothing to report in the uploaded pdf (see accomplishments).